Coupled-channel version of PT-symmetric square well

Miloslav Znojil

Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic[1]

Abstract

Coupled pair of PT-symmetric square wells is studied as a prototype of a quantum system characterized by two manifestly non-Hermitian commuting observables. Via the diagonalization of our Hamiltonian $H \neq H^\dagger$ and spin-like observable $\Omega \neq \Omega^\dagger$ we demonstrate that there exists a domain of couplings where both the respective sets of eigenvalues E_n, $n = 0, 1, \ldots$ (energies) and $\sigma = \pm 1$ ("spin projections") remain *real*. In such a "measurable" regime the model acquires a consistent probabilistic interpretation mediated by our selection of one of many available interaction-dependent scalar products.

PACS
03.65.Ca 03.65.Ge;

[1]e-mail: znojil@ujf.cas.cz

1 Introduction

One of the keys to the proposal of PT-symmetric Quantum Mechanics (PTSQM) by Bender and Boettcher [1] lied in the reality of the spectrum of the imaginary one-dimensional oscillator well $V_{(cubic)}(x) \sim ix^3$. Although the rigorous confirmation of that fundamental as well as phenomenologically welcome property of the model has been delivered a few years later [2], the proof remains rather abstract and complicated [3]. For this reason, a lot of parallel attention has been paid to the other, exactly solvable non-Hermitian potentials with real spectra [4]. People studied partially solvable (often called quasi-exact) analytic alternatives to $V_{(cubic)}(x) \sim ix^3$ [5] as well as non-analytic square-well potentials of similar type [6] and their singular point-interaction limits [7].

Solvable choices proved particularly suitable for illustrative purposes. Their study clarified that PTSQM formalism may be understood as a very natural extension of Quantum Mechanics, not asking for any new formulation of the "first principles". For a review we may recommend the recent dedicated Workshops' proceedings [8].

We intend to broaden the scope of the current PT-symmetric models beyond their popular ordinary differential equation (ODE) framework. We feel motivated by the observation that the majority of existing applications of the innovative PTSQM formalism concerns systems characterized by a *single* physical observable. We intend to fill the gap by an introduction of a model possessing a doublet of commuting independent observables (sect. 2). Our square-well-type model is solvable and intuitively transparent (sect. 3). It exemplifies a number of generic features of PTSQM systems (cf. discussion in sect. 4). Its appeal and properties are summarized in sect. 5.

A number of technical details is separated in Appendices A (an account of the perturbation representation of energies), B (summarizing the PTSQM formulism in a modified Dirac's notation), C (on norms) and D (on the single-channel projection).

2 The model

2.1 $\mathcal{PT}$−symmetry and its generalizations

The productivity of the counterintuitive PTSQM approach has been mainly revealed via studies of specific, concrete examples. Many of them proved too exceptional. Typically, one may recollect the elementary, exactly solvable spiked harmonic oscil-

lator of ref. [9] with its complete confluence of all the infinitely many 'exceptional points' defined as the couplings at which two neighboring real energies merge and complexify [10].

Among the less exceptional toy models, many conjectures have been deduced from discontinuous solvable potentials. The simplest, purely imaginary piece-wise constant potential of ref. [6] with single discontinuity contributed to our understanding of the mechanisms of stabilization of the real spectra [11]. Supersymmetric partners of this potential have been found obtainable by non-numerical means [12]. The study of its physical aspects and classical limit proved facilitated by its perturbative tractability [13]. A model-independence of most of these observations was confirmed by the long-range square-well model with two discontinuities [14], by the short-range model with three discontinuities [15] and by the harmonic oscillator decorated with two delta-function discontinuities [16].

All the above-mentioned solvable models offered an independent support for the inspiring conjecture of ref. [1] that the reality of spectra is related to the so called PT-symmetry of the potentials. This connects the observed absence of the complex energy eigenvalues with the invariance of the Hamiltonians with respect to the combined action of a complex conjugation $\mathcal{T}$ and a parity reversal $\mathcal{P}$, $\mathcal{PT}H = H\mathcal{PT}$ (cf. ref. [17]).

The latter type of symmetry gave its name to all the PTSQM formalism. Beyond the simplest ODE Hamiltonians, the emphasis on the parity and time reversal meaning of the operator $\mathcal{PT}$ may be weakened [18]. Thus, the parity $\mathcal{P}$ may be replaced by an arbitrary invertible self-adjoint operator P or, in a less confusing notation, θ. In parallel, the meaning of the complex conjugation $\mathcal{T} = \mathcal{T}^{-1}$ may be extended to all the Hermitian-conjugation involutions $A \to A^\dagger = \mathcal{T}A\mathcal{T}^{-1}$ [19]. The PTSQM concepts become applicable to nonsymmetric operators and the PT-symmetry becomes re-interpreted as the property

$$H^\dagger = \theta\, H\, \theta^{-1}, \qquad \theta = \theta^\dagger \tag{1}$$

called $\theta-$pseudo-Hermiticity of H [20].

An appreciation of the subtlety of the latter generalization requires a non-ODE model possessing more than one observable. We intend to describe here such a model in detail.

2.2 Two coupled channels

The frequent use of the coupling of channels in physics [21, 22] attracted our attention to the partitioned

$$\theta = \theta^\dagger = \left(\begin{array}{cc} 0 & \mathcal{G} \\ \mathcal{G} & 0 \end{array} \right), \qquad \theta^{-1} = \left(\begin{array}{cc} 0 & \mathcal{G}^{-1} \\ \mathcal{G}^{-1} & 0 \end{array} \right) \tag{2}$$

with any parity-type invertible sub-operator $\mathcal{G} = \mathcal{G}^\dagger$ which is not necessarily involutive.

A coupled pair of equal-mass particles moving in single spatial dimension inside a deep square-well box will be considered, exhibiting the symmetry (1) + (2) of their non-Hermitian Hamiltonian $H = H_{(kinetic)} + H_{(interaction)}$. In units $\hbar = 2m = 1$ we shall have

$$H_{(kinetic)} = \left(\begin{array}{cc} -\frac{d^2}{dx^2} & 0 \\ 0 & -\frac{d^2}{dx^2} \end{array} \right), \qquad H_{(interaction)} = \left(\begin{array}{cc} V_a(x) & W_b(x) \\ W_a(x) & V_b(x) \end{array} \right). \tag{3}$$

The pseudo-metric (2) commutes with the kinetic (i.e., differential) operator $H_{(kinetic)}$ so that the $\theta-$pseudo-Hermiticity condition (1) will degenerate to an explicit definition of $V_b = \mathcal{G}^{-1} V_a^\dagger \mathcal{G}$ and to the two $\mathcal{G}-$pseudo-Hermiticity relations

$$W_a^\dagger = \mathcal{G} W_a \mathcal{G}^{-1}, \qquad W_b^\dagger = \mathcal{G} W_b \mathcal{G}^{-1}.$$

Although we emphasized the generality of the operator $\mathcal{G}$ acting in the single-channel subspace, we shall simplify the discussion by a return to the common parity reversal in what follows, $\mathcal{G} = \mathcal{P}$.

In order to select a specific channel-coupling interaction in (3) we shall pick up a maximally simplified, purely imaginary piece-wise-constant potential such that $\mathrm{Re}\, V_{a,b}(x) = \mathrm{Re}\, W_{a,b}(x) = 0$ and

$$\begin{array}{l} \mathrm{Im}\, W_a(x) = X > 0, \qquad \mathrm{Im}\, W_b(x) = Y > 0, \qquad x \in (-1, 0), \\ \mathrm{Im}\, W_a(x) = -X, \qquad \mathrm{Im}\, W_b(x) = -Y, \qquad x \in (0, 1), \\ \mathrm{Im}\, V_a(x) = \mathrm{Im}\, V_b(x) = Z, \qquad x \in (-1, 0), \\ \mathrm{Im}\, V_a(x) = \mathrm{Im}\, V_b(x) = -Z, \qquad x \in (0, 1). \end{array} \tag{4}$$

This non-Hermitian model of the coupling of channels is defined in terms of its three real parameters X, Y and Z. This represents an immediate generalization of the single-channel square well of ref. [6] in which the spectrum happened to be real at all the not too large coupling constants [23]. Basically, we intend to prove the same for eq. (4).

3 Solutions

3.1 Non-Hermitian symmetry Ω

Hamiltonian H of eq. (3) enters the coupled-channel Schrödinger equation

$$H \left(\begin{array}{c} \varphi(x) \\ \chi(x) \end{array} \right) = E \left(\begin{array}{c} \varphi(x) \\ \chi(x) \end{array} \right) . \tag{5}$$

It specifies the bound states of the model when accompanied by the current asymptotic boundary condition re-scaled to $L = 1$,

$$\left. \left(\begin{array}{c} \varphi(x) \\ \chi(x) \end{array} \right) \right|_{x=\pm L} = \left(\begin{array}{c} 0 \\ 0 \end{array} \right) . \tag{6}$$

A merit of such a choice of the example is that its two-by-two Hamiltonian of eq. (3) commutes with the spin-like constant matrix

$$\Omega = \left(\begin{array}{cc} 0 & \omega^{-1} \\ \omega & 0 \end{array} \right) , \qquad \omega = \sqrt{\frac{X}{Y}} > 0.$$

It plays the role of another non-Hermitian "observable". Its eigenvalues $\sigma = \pm 1$ are real and it exhibits also the $\theta-$pseudo-Hermiticity property,

$$\Omega^\dagger = \theta \Omega \theta^{-1}.$$

The existence of the symmetry Ω implies that Schrödinger equation (5) may be complemented by the fixed-spin constraint

$$\Omega \left(\begin{array}{c} \varphi_\sigma(x) \\ \chi_\sigma(x) \end{array} \right) = \sigma \left(\begin{array}{c} \varphi_\sigma(x) \\ \chi_\sigma(x) \end{array} \right) . \tag{7}$$

It gives the relation between the channels at both the spin eigenvalues $\sigma = \pm 1$,

$$\chi_\sigma(x) = \sigma \omega \varphi_\sigma(x). \tag{8}$$

For the sake of brevity we shall mostly drop the subscripts $_\sigma$ in what follows.

3.2 Wavefunctions

The connection (8) between the channels reduces the system of equations (5) into the *single*, $\sigma-$dependent linear differential equation with the piece-wise constant coefficients,

$$-\frac{d^2}{dx^2}\varphi_n(x) + \left[V_a(x) + \sigma\omega W_b(x)\right]\varphi_n(x) = E_n \varphi_n(x), \qquad x \in (-1, 1). \tag{9}$$

The necessary incorporation of the "asymptotic" boundary conditions (6) reduces further its general solutions to the ansatz

$$\varphi(x) = \begin{cases} A \sin \kappa_L(x+1), & x \in (-1,0), \\ C \sin \kappa_R(1-x), & x \in (0,1). \end{cases} \tag{10}$$

The insertion of this ansatz in eq. (9) gives the linear relations

$$E = \kappa_L^2 + \mathrm{i}(Z + \sigma\sqrt{XY}) = \kappa_R^2 - \mathrm{i}(Z + \sigma\sqrt{XY}) \tag{11}$$

which define the energy and connect κ_L with κ_R at any given, fixed value of $\sigma = \pm 1$.

Once we expect that the energies are observable we have to *assume* that all their values $E = E_n$ remain real. *Vice versa*, we are persuaded that for a certain fairly broad class of the coupled-channel non-Hermitian interactions and equations on a finite interval the *general* rigorous proof of the existence of a non-empty physical domain of parameters (where the energies remain real) may be based on the straightforward extension of the proof delivered by Langer and Tretter in the single-channel case [24]. For our present purposes we shall feel satisfied by the less ambitious approach paralleling simply the single-channel construction of ref. [6].

Within our physical domain $\mathcal{D}$ of the real X, Y, Z and E the inspection of eqs. (11) and (10) reveals that we may set $\kappa_L = \kappa_R^* = \kappa = s - \mathrm{i}t$. At a fixed spin σ this re-defines

$$E = s^2 - t^2, \qquad Z = 2st - \sigma\sqrt{XY} \tag{12}$$

in terms of some new pair of real parameters s and t. We may keep one of them positive (say, $s > 0$) while the second one lies on a branch of a hyperbolic curve,

$$t = t_\sigma(s) = \frac{1}{2s} Z_{eff}(\sigma), \qquad Z_{eff}(\sigma) = Z + \sigma\sqrt{XY}, \quad \sigma = \pm 1. \tag{13}$$

We see that the energies remain non-degenerate with respect to the spin σ in general.

The quantization will be mediated by the requirement of the continuity of the wave functions $\varphi(x)$ and $\chi(x)$ and of their first derivatives at $x = 0$. These conditions degenerate to the single pair of complex equations

$$A \sin \kappa = C \sin \kappa^*, \qquad A\kappa \cos \kappa = -C\kappa^* \cos \kappa^*.$$

The first item fixes the normalization ($A = C \sin \kappa^* / \sin \kappa$) while the elimination of C gives the complex constraint $\mathrm{Re}\,(\kappa^{-1} \tan \kappa) = 0$. It is equivalent to the single, $\sigma-$independent real secular equation

$$s \sin 2s + t \sinh 2t = 0. \tag{14}$$

Our construction of bound states is completed. They are determined by formulae (10) and (12) while their free parameters s and t must be fixed by the pair of eqs. (13) and (14). A few comments on the practical numerical and perturbative evaluation of the roots (s_n, t_n) may be found in Appendix A.

4 Interpretation of the solutions

One does not leave the Standard Textbook Quantum Mechanics (STQM) whenever feeling satisfied by the Hilbert space $\mathcal{H}_{(physical)}$ where the scalar product [i.e., metric operator Θ in its definition $(a, b)_{(physical)} = \langle a|\Theta|b\rangle$] is kept trivial, $\Theta_{(STQM)} \equiv I$. In contrast, one is allowed and advised to admit a nontrivial metric within PTSQM framework, $\Theta_{(PTSQM)} \neq I$ [25].

In the latter setting it is important to keep in mind that the non-Hermiticity of the operators of observables (i.e., of H and Ω in our present illustrative example) might lead to some confusion in the standard Dirac's 'bra-ket' notation. For this reason, the slightly modified 'brabra-ket' notation of ref. [22] is advocated and summarized here in Appendix B.

4.1 Physical metric Θ

The extended flexibility of PTSQM formalism is compensated by the necessity of an explicit construction of a consistent physical metric operator $\Theta_{(PTSQM)} \neq \theta$. It must be Hermitian ($\Theta = \Theta^\dagger$) and positive definite ($\Theta > 0$). The new freedom broadens the class of the observables $H = \mathcal{O}^{(j)}_{(PTSQM)}$, $j = 1, 2, \ldots, M$ which must be quasi-Hermitian, i.e., by definition, Hermitian in our new metric,

$$H^\dagger = \Theta\, H\, \Theta^{-1}. \tag{15}$$

According to the review paper [26] the introduction of the observables of this type may be made in a mathematically consistent as well as phenomenologically appealing manner. From a pragmatic point of view, it proved particularly productive in nuclear physics where $M > 1$ as a rule.

Requirement (15) looks difficult to satisfy, especially in less elementary quantum systems. The key to the *technical feasibility* of the transition STQM $\to$ PTSQM has been found in the existence of an indeterminate, *auxiliary* pseudo-metric P (renamed as θ, in our coupled-channel eq. (1), in an attempt to avoid its easy confusion

with a very similar symbol $\mathcal{P}$ for parity). This means that one should speak, strictly speaking, about a $\theta\mathcal{T}-$symmetric Quantum Mechanics throughout our text.

One usually proceeds in an opposite direction, from a (preferably, *very* simple) pseudo-metric to metric. Thus, a complete set of eigenstates of a given set of $\theta-$pseudo-Hermitian observables is constructed in the first step, and the proof of the reality of the energies is then added as quite a difficult task. In this sense, our present solvable model may serve as a source of an insight in the properties of the wavefunctions (cf. sect. 3.2) as well as of the domain of the reality of the spectrum (cf. Appendix A).

On this background let us now address the correct physical interpretation of the theory. It is to be achieved via a specification of the physical metric, *to be constructed* as a Hermitian and positive definite *solution* $\Theta = \Theta^\dagger > 0$ of eq. (15). Its knowledge will enable us to treat any quasi-Hermitian operator A with the property $A^\dagger = \Theta\, A\, \Theta^{-1}$ as an observable.

Once we start from the spectral representation (32) of H (cf. Appendix B), we may recall the property $H^\dagger\Theta = \Theta H$ and infer that

$$\Theta = \sum_{E,\,\sigma,\,F,\,\tau} |F,\tau\rangle\!\rangle\; S_{F,\tau,\,E,\,\sigma}\; \langle\!\langle E,\sigma|\,. \tag{16}$$

The choice of the expansion coefficients S must remain compatible with eq. (15) and with the symmetry Ω. This gives the conditions

$$S_{E,\sigma,\,F,\,\tau}\;\,(E^* - F) = 0, \qquad S_{E,\sigma,\,F,\,\tau}\;\,(\sigma - \tau) = 0.$$

The spectrum of energies is assumed real so that the off-diagonal part of the array S must vanish. We may replace the quadruple sum (16) by the double-sum ansatz

$$\Theta = \sum_{n,\,\sigma} |E_n,\sigma\rangle\!\rangle\; S_{n,\,\sigma}\; \langle\!\langle E_n,\sigma|\,. \tag{17}$$

It represents the formal solution of eq. (15) and contains the infinite sequence of arbitrary coefficients $S_{n,\,\sigma}$. Whenever they do not vanish, $S_{n,\,\sigma} \neq 0$, the operator (17) is formally invertible,

$$\Theta^{-1} = \sum_{n,\,\sigma} |E_n,\sigma\rangle\; \frac{1/S_{n,\,\sigma}}{\langle E_n,\sigma|E_n,\sigma\rangle\!\rangle \cdot \langle\!\langle E_n,\sigma|E_n,\sigma\rangle}\; \langle E,\sigma|\;.$$

The necessary [26] Hermiticity of Θ is guaranteed when all the parameters $S_{n,\,\sigma}$ remain real. The necessary positivity of Θ (which means its tractability as a genuine physical metric) will be achieved whenever all the coefficients remain positive, $S_{n,\,\sigma} > 0$.

We see that the acceptable metric (17) compatible with all the standard physical requirements exists (at least in the formal sense) and is non-unique. One is allowed to impose some other mathematical or physical requirements [18, 27].

4.2 Normalization conventions and the norm

In our bound-state solutions $|E_n, \sigma\rangle$ of eq. (10) we are free to use any complex 'normalization' constants $C = C_{n,\sigma}$. The same freedom of choice applies to another series of the 'normalization' constants which would appear in the similar formulae for the 'left' eigenkets $\langle\!\langle E_n, \sigma|$. This is unaffected by the observation of Appendix B that the respective definitions (29) and (30) are connected by the pseudo-Hermiticity property (1). One can only conclude that in all the non-degenerate cases the following proportionality rule remains valid,

$$|E, \sigma\rangle \sim \theta^{-1}\, |E^*, \sigma^*\rangle\!\rangle.$$

For $E = E^*$ and $\sigma = \sigma^*$ at $Z < Z_{crit}$ we may treat the latter rule as a *definition* of the eigenkets $|\cdot, \cdot\rangle\!\rangle \in \mathcal{H}$ up to a normalization,

$$|E, \sigma\rangle\!\rangle = \theta\, |E, \sigma\rangle\, \varrho_{E\sigma}^{(optional)}, \qquad E = E_0, E_1, \ldots = \text{real}, \qquad \sigma = \pm 1. \tag{18}$$

The explicit solution of the left eigenproblem (30) is made redundant but the freedom in the choice of a convenient relative normalization (RN) factor $\varrho_{E\sigma}^{(optional)}$ survives.

The same factor emerges in the following formula for the overlaps between eigenstates,

$$\langle\!\langle E_{n'}, \sigma'|E_n, \sigma\rangle = \delta_{\sigma\sigma'}\delta_{nn'}\, \varrho_{E_n\sigma}^{(optional)}\, \langle E_n, \sigma|\, \theta\, |E_n, \sigma\rangle\,, \qquad n, n' = 0, 1, \ldots, \qquad \sigma, \sigma' = \pm 1. \tag{19}$$

Before its deeper analysis one may consult Appendix C which shows how our coupled-channel Hilbert space $\mathcal{H}$ may be partitioned into two single-channel subspaces $\mathcal{H}_c$. This partitioning is prescribed there in such a way that our (free) choice of an overall normalization coefficient entering the right eigenstate $|E_n, \sigma\rangle$ is unambiguously inherited by its single-channel components $|\varphi_n\rangle$ via eq. (33). In parallel, an *independent* choice of the coefficient in each left eigenstate $\langle\langle E_n, \sigma|$ is transferred to its single-channel components by eq. (34).

On this background we must inter-relate our full-space and subspace RN conventions. The factor $\varrho_{E_n\sigma}^{(optional)}$ introduced in the full space $\mathcal{H}$ may differ from its subspace

partner $\lambda_{E_n\sigma}^{(optional)}$ of eq. (35). By construction, fortunately, both these quantities happen to coincide [cf. eq. (37) and the rest of Appendix C for more details of the proof]. As a consequence, the partitioning enables us to replace the non-vanishing overlaps in (19) by the much simpler matrix elements (36).

An inspection of the formulae (19) and (36) reveals that the absolute value of the self-overlap $\langle\!\langle E,\sigma|E,\sigma\rangle$ may be re-scaled to one by an appropriate choice of the 'normalization' constants $C = C_{n,\sigma}$ in eq. (10). We also restrict the RN factors by the similar condition while their sign remains free, $\varrho_{E_n\sigma}^{(optional)} = \pm 1$. The key consequence lies in the fact that the sign of all the non-vanishing self-overlaps (36) is *fully* controlled by the sign of our optional RN factor. In an opposite direction, we have a *freedom to prescribe* such a specific set $\varrho_{E_n\sigma}^{(special)} = \pm 1$ which guarantees the *positivity* of all the 'special' self-overlaps. Thus, in the light of eq. (36) we simply postulate $\langle\!\langle E_n,\sigma|E_n,\sigma\rangle_{(special)} > 0$, i.e.,

$$\sigma\, \varrho_{E_n,\sigma}^{(special)}\, \langle n|\mathcal{P}|n\rangle > 0\,. \tag{20}$$

After one evaluates the matrix element, this equation defines the *dynamically determined* "physical" RN factors which make our basis biorthonormal,

$$\langle\!\langle E_{n'},\sigma'|E_n,\sigma\rangle_{(special)} = \delta_{\sigma\sigma'}\delta_{nn'}\,.$$

The (positive-definite) "physical" norm

$$\|\,|E_n,\sigma\rangle\|_{(physical)} = \sqrt{\langle\!\langle E,\sigma|E,\sigma\rangle_{(special)}}$$

of our bound states is obtained as a byproduct. This definition may be extended to all the elements of $\mathcal{H}$ via completeness relations (31) [18, 20, 28].

4.3 Quasi-parity $\mathcal{Q}$

In the literature people call the re-scaled RN coefficients a "charge" [18] or "quasi-parity" [29]. It is important to notice that in our present example their explicit determination is not difficult since the matrix elements $\langle n|\mathcal{P}|n\rangle$ may be evaluated in closed form. Due to the purely trigonometric character of the wavefunctions (10) we have

$$\frac{1}{AA^*}\,\langle n|\mathcal{P}|n\rangle = \int_{-1}^{0} \sin\kappa^*(x+1)\sin\kappa(-x+1)\,dx + \int_{0}^{1} \sin\kappa(-x+1)\sin\kappa^*(x+1)\,dx =$$

$$= \frac{1}{2s} \sin 2s \,\text{cosh}2t - \frac{1}{2t} \cos 2s \,\text{sinh}2t \,.$$

The $n-$dependence of this element is particularly transparent at the higher excitations with large $s = \mathcal{O}(n)$ and small $|t| = \mathcal{O}(1/n)$. Our exact formula degenerates to its leading-order estimate

$$\frac{1}{AA^*} \langle n|\mathcal{P}|n\rangle = -\cos 2s + \mathcal{O}\left(\frac{1}{n}\right) = (-1)^n \cos Q_n + \mathcal{O}\left(\frac{1}{n}\right) = (-1)^n + \mathcal{O}\left(\frac{1}{n}\right) .$$

Thus, the "charge" or "quasi-parity" is specified by the closed formula

$$\varrho^{(special)}_{E_n \sigma} = (-1)^n \sigma, \qquad \sigma = \pm 1, \qquad n \gg 1$$

at the higher excitations.

Quasi-parities may now be interpreted as eigenvalues of a certain operator $\mathcal{Q}$,

$$\mathcal{Q}|E_n, \sigma\rangle = |E_n, \sigma\rangle \, \varrho^{(special)}_{E_n \sigma} \,. \tag{21}$$

We insert eq. (21) in (18) and deduce that

$$\langle\!\langle E_{n'}, \sigma'|E_n, \sigma\rangle_{(special)} = \langle E_{n'}, \sigma'|\theta \, \mathcal{Q}|E_n, \sigma\rangle, \qquad n, n' = 0, 1, \ldots, \qquad \sigma, \sigma' = \pm 1. \tag{22}$$

This identification defines an overlap of *two different* vectors using a specific scalar product in $\mathcal{H}$. In the light of sect. 4.1 such a particular product corresponds to a particular metric operator,

$$\Theta_{(particular)} = \theta \, \mathcal{Q}.$$

Combining this relation with eq. (17) we get

$$S^{(special)}_{n,\sigma} = \frac{1}{\langle\!\langle E_n, \sigma|E_n, \sigma\rangle_{(special)}} \,. \tag{23}$$

Vice versa, the violation of the one-to-one correspondence (23) between the metric and norm would require an "artificial" introduction of an $n-$ and $\sigma-$dependence into our definition (21) of the operator $\mathcal{Q}$. In spite of some formal merits of such a step [13] we are persuaded that the related "anisotropy" of both the operators $\mathcal{Q}$ and $\Theta_{(particular)}$ could hardly find a natural physical foundation.

4.4 The crossings and degeneracies of levels

Although the Hamiltonian H and "spin" Ω (and wavefunctions) of our model depend on three parameters, its energy spectrum itself feels merely the influence of Z and

of the product XY. In the light of eq. (28) the two sources of non-Hermiticity are the "internal" strength Z and the "coupling" strength $\sqrt{XY}$. Still, the distinction between X and Y is nontrivial. At $X = Y \neq 0$ giving a "symmetrized" coupling of channels, the operator of symmetry Ω becomes, incidentally, Hermitian.

A strongly asymmetric decoupling of our model may be achieved by the two alternative limiting transitions, viz., $Y \neq 0$, $X \to 0$ and $X \neq 0$, $Y \to 0$. Each of them suppresses just one of the channels [cf. (33)]. In both these limits the symmetry Ω ceases to exist. One gets $\omega \to \infty$ or $1/\omega \to \infty$ and our present method of solution becomes inapplicable.

A much more interesting limiting transition $Z \to 0$ (from both sides, i.e., $Z \to 0^+$ and $Z \to 0^-$) converts our model into a coupled set of two *Hermitian* square wells. In this limit the violation of the Hermiticity of the whole system is merely caused by the channel-coupling terms. The energies $E = s^2 - t^2$ degenerate with respect to the spin since $t_\sigma(s) = \sigma\, |t_\sigma(s)|$ so that, in fact, the neighboring $\sigma = \pm 1$ levels cross at $Z = 0$. No point of the crossing is "exceptional" since the corresponding wavefunctions remain linearly independent. Their Wronskian $\mathcal{W}$ does not vanish and both our observables H and Ω remain diagonalizable. In contrast to some other solvable examples (say, to the harmonic oscillator of ref. [9]), no Jordan-block structures emerge in H.

For the sufficiently small Z_{eff}, all the similar observations may be made quantitative. Taking the ground-state $n = 0$ and setting $Z_{eff} = \mathcal{O}(\lambda)$ while $Z = \mathcal{O}(\lambda^2)$ for definiteness, we deduce that $t = \mathcal{O}(\lambda)$ [cf. eq. (13)]. Next we convert eq. (14) with $s = \pi/2 + \varepsilon$ and a small $\varepsilon = \varepsilon_0$ [cf. eq. (24) in Appendix A] in the leading-order estimate of $\varepsilon = 4t^2/\pi + \ldots$. All this transforms the definition of the energy into the following approximate formula

$$E_0 = s_0^2 - t_0^2 = \frac{\pi^2}{4} + \frac{3XY}{\pi^2} - \sigma\, Z\, \frac{6\sqrt{XY}}{\pi^2} + \mathcal{O}\left(\lambda^4\right).$$

As long as $t_\sigma(s) = \sigma\, |t_\sigma(s)|$, the ground state has the "spin" $\sigma = +1$ at $Z > 0$ and $\sigma = -1$ at $Z < 0$ while it becomes doubly degenerate at $Z = 0$. At this point the Wronskian easily evaluates to a nonvanishing constant, $\mathcal{W} = AC\kappa^* \sin 2\kappa^*$. Hence, the two lowest states remain linearly independent at $Z = 0$.

5 Summary

The appeal of virtually all the PTSQM constructions may be seen in a universality of their transition from a simple though indefinite pseudometric θ to the correct physical and dynamically determined positive-definite metric Θ. The procedure is counterintuitive and a number of open questions emerges. We designed our present less trivial coupled-channel example to clarify some mathematical subtleties (like the necessary conditions of the reality of the spectrum in non-Hermitian models), a deeper understanding of which requires, typically, a nontrivial application of the Krein-space theory [24].

We believe that the explanation of many interrelated subtleties of the PTSQM recipe may be facilitated via square-well models which offer one of the most economical combinations of a transparent dynamical picture with an exact solvability of the underlying equations based on the usual matching technique. Our specific present example illustrates, first of all, a phenomenologically important situation where the dynamics is controlled by *more* observable quantities.

An unexpected merit of our model has been found in a quick convergence of the auxiliary perturbation expansions of its energy-level parameters $s = s_n$ (such that $E = s^2 - const/s^2$) in the weak-coupling regime (i.e., for small strengths of the non-Hermiticity $|Z|$ and $|XY|$) and/or in the quasi-classical regime (i.e., at the higher excitations with $n \gg 1$). Another, highly welcome byproduct of the square-well solvability emerged as a non-Hermitian spin-type symmetry Ω of H. It enabled us to reduce our nontrivial (viz., coupled-channel) Schrödinger equation to its much more easily tractable "model-space" reduction. In parallel, the existence of the symmetry enabled us to analyze a level-degeneracy and level-crossing phenomena in a neat, non-numerical manner.

The elementary algebraic structure of our model facilitated a clarification of one of the most puzzling PTSQM requirements of keeping *all* the observables $\Theta-$quasi-Hermitian and, at the same time, $\theta-$pseudo-Hermitian in the Hilbert space $\mathcal{H}$. The coupled-channel (i.e., partitioned) structure of the model enabled us to clarify the mechanism of this correspondence anew. In particular, we showed that the quasi-parity-based factorization $\Theta = \theta\mathcal{Q}$ as introduced in ref. [28] appears mathematically more natural than the alternative charge-based factorization $\Theta = \mathcal{C}P$ of ref. [18], with $P = \theta$ in our present notation. Indeed, while the quasi-parity is a symmetry of the Hamiltonian itself (we have $[H, \mathcal{Q}] = 0$), the formally equivalent introduction of

the charge $\mathcal{C}$ in [18] implies that $[H^\dagger, \mathcal{C}] = 0$. This means that the charge is merely a symmetry of an operator $H^\dagger \neq H$ defined as a Hermitian-conjugate partner of the Hamiltonian.

Due to the existence of the second, $\theta-$pseudo-Hermitian and $\Theta-$quasi-Hermitian spin-like observable Ω in our model, another persuasive manifestation of a deep relevance of the symmetries of H has been revealed in the interrelations between the full space Hilbert space $\mathcal{H}$ and its reduced, single-channel subspace $\mathcal{H}_c$. *Pars pro toto*, the quasi-parity-related factorization $\Theta = \theta\mathcal{Q}$ of the metric in full space $\mathcal{H}$ has been proved accompanied by its analogue (40) using two relative quasi-parities $\mathcal{R}(\sigma)$ defined within the single-channel subspace $\mathcal{H}_c$.

The idea of the coupling of channels may turn attention to the systems treated perturbatively in more dimensions [30] as well as to non-perturbative explanations of the observed transitions between regular and chaotic classical and quantum motion controlled by the partial differential equations (PDE) [31]. Via our example, some existing confirmations of the internal consistency of the PTSQM theory may find their extension to the coupled-channel scenario. On this basis, "next" moves in the PTSQM development may be predicted as aiming at the non-separable PDE models [32] where some aspects of our model might inspire a more intensive exploration of the level-degeneracy patterns in non-Hermitian context [33] etc.

Acknowledgement

Work supported by the grant Nr. A 1048302 of GA AS CR.

References

[1] Bender C M and Boettcher B 1998 Phys. Rev. Lett. 80 4243;

Bender C M, Boettcher S and Meisinger P N 1999 J. Math. Phys. 40 2201

[2] Dorey P, Dunning C and Tateo R 2001 J. Phys. A: Math. Gen. 34 5679

[3] Alvarez G 1995 J. Phys. A: Math. Gen. 27 4589;

Shin K C 2001 J. Math. Phys. 42 2513;

Mostafazadeh A 2005 J. Phys. A: Math. Gen. 38 6557

[4] Andrianov A A, Cannata F, Dedonder J-P and Ioffe M V 1999 Int. J. Mod. Phys. A 14 2675;

Lévai G and Znojil M 2000 J. Phys. A: Math. Gen. 33 7165

[5] Bender C M and Boettcher S 1998 J. Phys. A: Math. Gen. 31 L273;

Znojil M 2000 J. Phys. A: Math. Gen. 33 4203;

Bagchi B, Cannata F and Quesne C 2000 Phys. Lett. A 269 79

[6] Znojil M 2001 Phys. Lett. A. 285 7

[7] Hernández E, Jáuregui A and A Mondragón A 2000 J. Phys. A: Math. Gen. 33 4507;

Albeverio S, Fei S-M and Kurasov P 2002 Lett. Math. Phys. 59 227;

Weigert S 2004 Czech. J. Phys. 54 1139;

Znojil M and Jakubský V 2005 J. Phys. A: Math. Gen. 38 5041;

Fei S-M 2005 Czech. J. Phys. 55 1085

[8] dedicated January and October issues: 2004 Czech. J. Phys. 54, pp. 1 - 156 and 1005 - 1148 and

dedicated September issue: 2005 Czech. J. Phys. 55, pp. 1045 - 1192

[9] Znojil M 1999 Phys. Lett. A 259 220

[10] Dembowski C et al 2001 Phys. Rev. Lett. 86 787;

Heiss W D and Harney H L 2001 Eur. Phys. J. D 17 149;

Günther U and Stefani F 2005 Czech. J. Phys. 55 1099

[11] Znojil M 2004 J. Math. Phys. 45 4418

[12] Bagchi B, Mallik S and Quesne C 2002 Mod. Phys. Lett. A 17 1651;

[13] Mostafazadeh A and Batal A 2004 J. Phys. A: Math. Gen. 37 11645

[14] Znojil M 2005 J. Math. Phys. 46 062109

[15] Quesne C et al 2005 Czech. J. Phys. 55 1161

[16] Demiralp E 2005 Czech. J. Phys. 55 1081

[17] Buslaev V and Grecchi V 1993 J. Phys. A: Math. Gen. 26 5541

[18] Bender C M, Brody D C and Jones H F 2002 Phys. Rev. Lett. 89 0270401;

Kleefeld F 2003 AIP conf. proc. 660 325;

Znojil M 2004 hep-th/0408081 in "Symmetry Methods in Physics", CD ROM proc. series, Ed. C. Burdik, O. Navratil and S. Posta (Dubna: JINR)

[19] Mostafazadeh A 2003 LANL quant-ph/0310164;

Bender C M, Brody D C and Jones H F 2004 Phys. Rev. Lett. 92 0119902 (erratum)

[20] Mostafazadeh A 2002 J. Math. Phys. 43 205

[21] Vanroose W, Van Leuven P, Arickx F and Broeckhove J 1997 J. Phys. A: Math. Gen. 30 5543;

Mostafazadeh A 2003 Class. Quantum Grav. 20 155

[22] Znojil M 2004 J. Phys. A: Math. Gen. 37 9557

[23] Znojil M and Lévai G 2001 Mod. Phys. Letters A 16 2273;

Jakubský V and Znojil M 2004 Czech. J. Phys. 54 1101;

Weigert S 2005 Czech. J. Phys. 55 1183

[24] Langer H and Tretter C 2004 Czech. J. Phys. 54 1113

[25] Mostafazadeh A 2002 J. Math. Phys. 43 2814 and 3944

[26] Scholtz F G, Geyer H B and Hahne F J W 1992 Ann. Phys. (NY) 213 74

[27] Geyer H B, Scholtz F G and Snyman I 2004 Czech. J. Phys. 54 1069;

Kretschmer R and Szymanowski L 2004 Phys. Lett. A 325 112

[28] Znojil M 2001 LANL report math-ph/0104012, reprinted 2004 Rendiconti del Circ. Mat. di Palermo, Ser. II, Suppl. 72 211

[29] Bagchi B and C. Quesne C 2000 Phys. Lett. A 273 285;

Bagchi B, Quesne C and Znojil M 2001 Mod. Phys. Lett. A 16 2047;

Sinha A and Roy P 2004 Czech. J. Phys. 54 129

[30] Caliceti E 2004 Czech. J. Phys. 54 29;

Caliceti E 2005 Czech. J. Phys. 55 1077

[31] Ahmed Z and Jain S R 2003 Phys. Rev. E 67 R045106;

Nanayakkara A and Abayaratne Ch 2003 Can. J. Phys. 81 835

[32] Znojil M and Tater M 2001 J. Phys. A: Math. Gen. 34 1793;

Bender C M, Dunne G V, Meisinger P N and Simsek M 2001 Phys. Lett. A 281 311;

Basu-Mallick B, Bhattacharyya T, Kundu A and Mandal B P 2004 Czech. J. Phys. 54 5;

Jakubský V 2004 Czech. J. Phys. 54 67

[33] Nanayakkara A 2005 Phys. Lett. A 334 144;

Bíla H, Tater M and Znojil M 2005 Phys. Lett. A., Comment, submitted

[34] Caliceti E, Graffi S and Maioli M 1980 Commun. Math. Phys. 75 51;

Fernández F M, Guardiola R, Ros J and Znojil M 1998 J. Phys. A: Math. Gen. 31 10105;

Bender C M 2004 Czech. J. Phys. 54 1027;

Bíla H 2004 Czech. J. Phys. 54 1049;

Jones H F 2004 Czech. J. Phys. 54 1107

Appendices

A. Perturbation series for the energies

PTSQM models usually require some sufficiently efficient numerical description which is, typically, perturbative [34]. It may mediate an alternative or quicker insight even in the solvable models. *Vice versa*, the exact solvability of our present model offers an explicit verification of the approximative approaches.

The predominantly trigonometric oscillatory character of the functions entering our secular eq. (14) enables us to locate and count all its physical roots,

$$s = s_n = \frac{(n+1)\pi}{2} + (-1)^n \frac{Q_n}{2}, \qquad n = 0, 1, \ldots \tag{24}$$

where the new parameter Q_n remains small in the weak-coupling regime (i.e., for all the sufficiently small X, Y and Z) as well as at all the sufficiently large n. This enables us to abbreviate

$$\frac{1}{(n+1)\pi} = \varrho \equiv \frac{1}{L}, \qquad \frac{2\, Z_{eff}(\sigma)}{L} = \alpha, \qquad \frac{2\, Z_{eff}(\sigma)}{L^2} = \beta = \alpha\varrho$$

and to re-write our secular eq. (14) in terms of these new "small" parameters and a sign factor $\tau = (-1)^n$,

$$Q = \arcsin\left(2t\, \frac{\varrho}{1+\tau\, Q\, \varrho}\, \sinh 2t\right), \qquad 2t = \frac{\alpha}{1+\tau\, Q\, \varrho}\,. \tag{25}$$

As long as

$$\arcsin(x) = x + \frac{1}{6}x^3 + \frac{3}{40}x^5 + \frac{5}{112}x^7 + \ldots$$

we may iterate eq. (25) and observe that the $\alpha-$ and $\beta-$dependence of $Q = Q(\alpha, \beta)$ must acquire the following general asymptotic-series form

$$Q = Q(\alpha, \beta) = \alpha\beta\, \Sigma(\alpha, \beta), \qquad \Sigma(\alpha, \beta) = \sum_{k,\ell=0}^{\infty} \alpha^{2k}\beta^{2\ell}\, c_{k\,\ell} \tag{26}$$

where $c_{0\,0} = 1$. In practice, this series should be truncated in α as well as in β or, equivalently, in ϱ. Nevertheless, as long as the size of $\beta = \varrho\alpha$ is dominated by α, it is sufficient to analyse this series as a power series expansion in the single "small" parameter α. It is also worth noting that at any fixed power of α there is always just a finite number of the related powers of ϱ.

For illustration, let us set

$$\Sigma(\alpha, \beta) = 1 + c_{10}\, \alpha^2 + c_{0\,1}\, \beta^2 + c_{20}\, \alpha^4 + c_{11}\, \alpha^2\beta^2 + c_{0\,2}\, \beta^4 + \mathcal{O}(\alpha^6)$$

and insert this formula in the re-arranged eq. (25),

$$[1+\tau\,\beta^2\Sigma(\alpha,\beta)]\,\text{arcsinh}\left\{[1+\tau\,\beta^2\Sigma(\alpha,\beta)]^2\,\frac{1}{\beta}\,\sin[\alpha\beta\,\Sigma(\alpha,\beta)]\right\}=\alpha\,. \tag{27}$$

As long as we can employ the regular Taylor series

$$\frac{1}{\beta}\,\sin[\alpha\beta\,\Sigma(\alpha,\beta)]=\alpha+\left(c_{10}+c_{01}\,\varrho^2\right)\alpha^3+\left[c_{20}+(c_{11}-1/6)\,\varrho^2+c_{02}\,\varrho^4\right]\alpha^5+\mathcal{O}\left(\alpha^7\right)$$

the left-hand side of eq. (27) evaluates to a power series in our small parameters. The tedious though straightforward calculation converts the resulting equation into the infinite series dominated by the leading-order identity

$$0=\left(-\frac{1}{6}+c_{10}+c_{0\,1}\,\varrho^2+3\,\tau\,\varrho^2\right)\alpha^3+\dots\,.$$

It determines the first two coefficients,

$$c_{10}=\frac{1}{6},\qquad c_{0\,1}=-3\tau\,.$$

Their insertion simplifies the next-order $O\left(\alpha^5\right)$ identity to the similar linear algebraic relation which defines the next set of the coefficients in $\Sigma(\alpha,\beta)$,

$$c_{20}=\frac{1}{120},\qquad c_{1\,1}=\frac{1-8\tau}{6},\qquad c_{0\,2}=15\,.$$

In this manner one may continue the construction of the solution (26) to an arbitrary order in α.

In the original notation we may now write down the second-order formula

$$Q_n=\frac{4\,Z_{eff}^2}{(n+1)^3\pi^3}+\frac{8\,Z_{eff}^4}{3\,(n+1)^5\pi^5}\left(1+\frac{18\,(-1)^{n+1}}{(n+1)^2\pi^2}\right)+\mathcal{O}\left(\frac{Z_{eff}^6}{(n+1)^7}\right)$$

etc. The convergence in $1/(n+1)$ is amazingly rapid and the role and weight of the non-Hermiticity decreases very quickly with the growth of the excitation n.

In the single-channel limit where $X=Y=0$ it has been observed that the growth of $|Z|=|Z_{eff}|$ makes some of the low-lying energies move towards each other. With the growth of the absolute value of Z they first pair (in fact, E_0 and E_1) merges and complexifies beyond the critical value of $Z_{crit}\approx 4.48$ [6, 23]. In the coupled-channel context we may repeat the same mathematical analysis leading, *mutatis mutandis*, to the conclusion that all the observable values of energies $E=E_n$ and quasi-spins σ remain real in the weakly non-Hermitian regime defined by the pair of inequalities $|Z_{eff}(\sigma)|<Z_{crit}$, $\sigma=\pm 1$. They may be compressed into single condition

$$\left|\sqrt{XY}\right|+|Z|<Z_{crit}\approx 4.48\,. \tag{28}$$

In contrast to the single-channel case, the energy spectrum now ceases to be real at $Z=\pm\left(Z_{crit}-\sqrt{XY}\right)$, i.e., along two distinct surfaces in the space of parameters.

B. Modified Dirac's notation

Our pair of operators H and Ω samples a complete set of non-Hermitian commuting observables. These operators enter Schrödinger eq. (5) with quasi-spin constraint (7), i.e., in the Dirac's notation, the pair of equations

$$H\,|E,\sigma\rangle = E\,|E,\sigma\rangle, \qquad \Omega\,|E,\sigma\rangle = \sigma\,|E,\sigma\rangle \tag{29}$$

As long as $H^\dagger \neq H$ and $\Omega^\dagger \neq \Omega$, the eigenkets $|\cdot,\cdot\rangle$ in (29) *differ* from the simultaneous eigenvectors of $H^\dagger$ and $\Omega^\dagger$. In the spirit of ref. [22] let us now adapt the Dirac's notation to the non-Hermitian scenario and equip the latter elements of our Hilbert space $\mathcal{H}$ by the double delimiter. The apparently unmotivated complex conjugation of the energies and spins in their implicit definition

$$H^\dagger\,|E,\sigma\rangle\!\rangle = E^*\,|E,\sigma\rangle\!\rangle, \qquad \Omega^\dagger\,|E,\sigma\rangle\!\rangle = \sigma^*\,|E,\sigma\rangle\!\rangle$$

becomes explained after the Hermitian conjugation which reveals the "left action" essence of these equations,

$$\langle\!\langle E,\sigma|\,H = E\,\langle\!\langle E,\sigma|, \qquad \langle\!\langle E,\sigma|\,\Omega = \sigma\,\langle\!\langle E,\sigma|\,. \tag{30}$$

For this reason we shall prefer the use of the ket-vector form of the 'right' eigenfunctions $|E,\sigma\rangle$ in combination with the doubly delimited (or 'brabra-vector') form $\langle\!\langle E,\sigma|$ of their 'left-eigenfunction' partners.

Although both the latter sequences of vectors are defined, strictly speaking, in the two equivalent copies of *the same* Hilbert space of states $\mathcal{H}$, our notation conventions will allow us to shorten the discussion here and there. As we already emphasized, our "redundant" version of the common Dirac's notation is transparent and proves more consistent in the non-Hermitian setting. Moreover, in the physical regime where $E = E^*$ and $\sigma = \sigma^*$ the two pairs of Schrödinger equations (29) and (30) imply the *biorthogonality* relations for their solutions which is easily written down now,

$$\langle\!\langle E',\sigma'|E,\sigma\rangle(E'-E) = 0, \qquad \langle\!\langle E',\sigma'|E,\sigma\rangle(\sigma'-\sigma) = 0.$$

In the general non-degenerate case these rules only admit the non-vanishing overlaps at $E' = E$ *and* $\sigma' = \sigma$. *Vice versa*, unless one of the self-overlaps vanishes accidentally, it is easy to derive the formal *completeness* relations

$$I = \sum_{E,\sigma}\,|E,\sigma\rangle\,\frac{1}{\langle\!\langle E,\sigma|E,\sigma\rangle}\,\langle\!\langle E,\sigma|\,. \tag{31}$$

Their use enables us to treat our set of two sequences of states $\langle\!\langle E,\sigma|$ and $|E,\sigma\rangle$ as a biorthogonalized basis giving straightforward formal expansions of any element $|\alpha\rangle \equiv I\cdot|\alpha\rangle \in \mathcal{H}$ or $|\beta\rangle\!\rangle \equiv I^\dagger\cdot|\beta\rangle\!\rangle \in \mathcal{H}$. Thus, one derives

$$H = \sum_{E,\sigma} |E,\sigma\rangle \frac{E}{\langle\!\langle E,\sigma|E,\sigma\rangle} \langle\!\langle E,\sigma|, \qquad \Omega = \sum_{E,\sigma} |E,\sigma\rangle \frac{\sigma}{\langle\!\langle E,\sigma|E,\sigma\rangle} \langle\!\langle E,\sigma| \tag{32}$$

as two samples of an extension of the usual *spectral representation* to (arbitrary) operators emerging in the non-Hermitian coupled-channel context. These formulae will be needed in sect. 4.1.

C. Partitioning of $\mathcal{H}$ into two subspaces $\mathcal{H}_c$

In eq. (19) we may employ the partitioned notation,

$$|E_n,\sigma\rangle = \left(\begin{array}{c} |\varphi_n\rangle\cdot\sqrt{Y} \\ |\varphi_n\rangle\cdot\sigma\sqrt{X} \end{array} \right), \qquad \sigma=\pm 1, \quad n=0,1,\ldots \tag{33}$$

where the subkets $|\varphi_n\rangle$ are $\sigma-$dependent solutions of eq. (9). In a left-action alternative to this formula let us put

$$\langle\!\langle E_n,\sigma| = \left(\sigma\sqrt{X}\,\langle\!\langle\chi_n|,\ \sqrt{Y}\,\langle\!\langle\chi_n|\right), \qquad \sigma=\pm 1, \quad n=0,1,\ldots \tag{34}$$

where the new subcomponents $\langle\!\langle\chi_n|$ are defined by a left-action version of eq. (9). More precisely, the left eigenstates $\langle\!\langle\chi_n|$ and the right eigenstates $|\varphi_n\rangle$ correspond to *the same* reduced and spin-dependent parity-pseudo-Hermitian single-channel sub-Hamiltonian

$$H(\sigma) = -\frac{d^2}{dx^2} + V_a + \sigma\omega W_b = \mathcal{P}\,H^\dagger(\sigma)\,\mathcal{P}$$

which acts in the single-channel Hilbert subspace $\mathcal{H}_c$ and which is, in the language of ref. [1], *truly* $\mathcal{PT}-$symmetric.

The partitioning clarifies the structure of the spectral representations of the operators in our basis. All of them may be derived from the elementary projectors

$$|E,\sigma\rangle\,\langle\!\langle E,\sigma| = \left(\begin{array}{cc} |\varphi_n\rangle\cdot\sigma\sqrt{XY}\cdot\langle\!\langle\chi_n| & |\varphi_n\rangle\cdot Y\cdot\langle\!\langle\chi_n| \\ |\varphi_n\rangle\cdot X\cdot\langle\!\langle\chi_n| & |\varphi_n\rangle\cdot\sigma\sqrt{XY}\cdot\langle\!\langle\chi_n| \end{array} \right)$$

entering, say, eq. (32). They may be understood as acting in two copies of $\mathcal{H}_c$ in $\mathcal{H} = \mathcal{H}_c \bigoplus \mathcal{H}_c$. We may abbreviate $|\varphi_n\rangle \equiv |n\rangle$ and $\langle\!\langle\chi_n| \equiv \langle\!\langle n|$ and collect the reduced Schrödinger equations,

$$H(\sigma)|n\rangle = E_n\,|n\rangle, \qquad \langle\!\langle n|\,H(\sigma) = E_n\,\langle\!\langle n|, \qquad n=0,1,\ldots\,.$$

They are to be solved in a single copy of $\mathcal{H}_c$ where their comparison leads to an alternative RN convention

$$|n\rangle\!\rangle = \mathcal{P}\,|n\rangle\,\lambda^{(optional)}_{E_n\sigma} \tag{35}$$

paralleling eq. (18). We must check that and how both these normalizations remain mutually compatible. For this purpose we start from the RN definition (18) and add the partitioning (33) or, alternatively, start from the partitioning (34) and insert the definition (35) afterwards. In the former case we proceed via eq. (19) and get

$$\langle\!\langle E,\sigma|E,\sigma\rangle = 2\sigma\,\left(\varrho^{(optional)}_{E_n\sigma}\right)^*\,\sqrt{XY}\,\langle n|\mathcal{P}|n\rangle\,. \tag{36}$$

In the latter case we have

$$\langle\!\langle E,\sigma|E,\sigma\rangle = 2\sigma\sqrt{XY}\,\langle\!\langle n|n\rangle = 2\sigma\,\left(\lambda^{(optional)}_{E_n\sigma}\right)^*\,\sqrt{XY}\,\langle n|\mathcal{P}|n\rangle\,.$$

A comparison of these two results reveals that

$$\lambda^{(optional)}_{E_n\sigma} \equiv \varrho^{(optional)}_{E_n\sigma}. \tag{37}$$

Our two apparently independent RN constants must be chosen equal to each other.

D. Quasi-parity in the subspaces $\mathcal{H}_c$

When we move to the single-channel subspace $\mathcal{H}_c$ we encounter the two different bases $\{\,|n\rangle\,\}$ distinguished by the "external" parameter σ. We have to fix $\sigma=+1$ or $\sigma=-1$ in $|n\rangle=|n_\sigma\rangle$. This means that in a sub-space analogue of eq. (21) we have to define the *two* "reduced quasi-parities" as operators $\mathcal{R}(\sigma)$ in $\mathcal{H}_c$ with a manifest dependence on the spin,

$$\mathcal{R}(\sigma)\,|n\rangle = \mathcal{R}(\sigma)\,|n_\sigma\rangle = |n\rangle\,\varrho^{(special)}_{E_n\sigma}\,.$$

At a fixed value of the spin σ we obtain a subspace counterpart of eq. (22),

$$\langle\!\langle n'_\sigma|n_\sigma\rangle_{(special)} = \langle n'_\sigma|\mathcal{P}\mathcal{R}(\sigma)|n_\sigma\rangle\,, \qquad n,n'=0,1,\ldots\,. \tag{38}$$

Although the spin-dependent product $\mathcal{P}\mathcal{R}(\sigma)$ plays just a not too important role of a subspace metric, its formal prolongation from $\mathcal{H}_c$ to the full space $\mathcal{H}$ is feasible and may be performed as follows. Firstly, one verifies that the action of the $\sigma-$dependent auxiliary operator

$$\mathcal{S}(\sigma) = \left(\begin{array}{cc} 0 & \sigma\omega^{-1}\,\mathcal{R}(\sigma) \\ \sigma\omega\,\mathcal{R}(\sigma) & 0 \end{array}\right) = \sigma\,\Omega\,\mathcal{R}(\sigma)$$

obeys the fixed-spin relation

$$\mathcal{S}(\sigma)\,|E_n,\sigma\rangle = \sigma\,\mathcal{R}(\sigma)\,|n\rangle\,\Omega\,\left(\begin{array}{c}\sqrt{Y}\\ \sigma\,\sqrt{X}\end{array}\right) = |E_n,\sigma\rangle\,\varrho^{(special)}_{E_n\sigma}\,.$$

A transition to the spin-independent formula will be then most naturally mediated by an introduction of the two two-by-two-matrix projectors $\Pi_\sigma = (I+\sigma\Omega)/2$,

$$\Pi_\sigma\,\mathcal{S}(\sigma)\,\Pi_\sigma|E_n,\sigma\rangle = |E_n,\sigma\rangle\,\varrho^{(special)}_{E_n\sigma}\,, \qquad \sigma=\pm1.$$

We may conclude that the spin-independent quasi-parity operator in the full space $\mathcal{H}$ may be *defined* by the formula $\mathcal{Q}=\sum_{\sigma=\pm1}\Pi_\sigma\,\mathcal{S}(\sigma)\,\Pi_\sigma$. In the partitioned notation we may re-write this operator in the matrix form,

$$\mathcal{Q} = \frac{1}{2}\left(\begin{array}{cc}\mathcal{R}(+1)+\mathcal{R}(-1) & \omega^{-1}\,[\mathcal{R}(+1)-\mathcal{R}(-1)]\\ \omega\,[\mathcal{R}(+1)-\mathcal{R}(-1)] & \mathcal{R}(+1)+\mathcal{R}(-1)\end{array}\right).$$

A return to another representation in terms of the projectors Π_σ is now possible,

$$\mathcal{Q} = \sum_{\sigma=\pm1}\mathcal{R}(\sigma)\,\Pi_\sigma\,. \qquad (39)$$

We see here that the two operators $\mathcal{R}(\sigma)$ may be perceived as representing "reduced" quasi-parities in $\mathcal{H}_c$. The new version of the factorization formula for the metric is delivered in the same spirit,

$$\Theta_{(special)} = \frac{1}{2}\left(\begin{array}{cc}\omega\,[\mathcal{P}\mathcal{R}(+1)-\mathcal{P}\mathcal{R}(-1)] & \mathcal{P}\mathcal{R}(+1)+\mathcal{P}\mathcal{R}(-1)\\ \mathcal{P}\mathcal{R}(+1)+\mathcal{P}\mathcal{R}(-1) & \omega^{-1}\,[\mathcal{P}\mathcal{R}(+1)-\mathcal{P}\mathcal{R}(-1)]\end{array}\right).$$

In the light of eq. (39) this formula represents our factorized metric $\Theta_{(special)}=\theta\,\mathcal{Q}$ as a weighted sum of two factorized items equipped with the appropriate spin projectors,

$$\Theta_{(special)} = \frac{1}{2}\sum_{\sigma=\pm1}\left(\begin{array}{cc}\sigma\omega & 1\\ 1 & \sigma\omega^{-1}\end{array}\right)\mathcal{P}\mathcal{R}(\sigma) = \sum_{\sigma=\pm1}\left(\begin{array}{cc}0 & \mathcal{P}\mathcal{R}(\sigma)\\ \mathcal{P}\mathcal{R}(\sigma) & 0\end{array}\right)\Pi_\sigma\,. \quad (40)$$

This conclusion is compatible with formulae (36) and (22).